

Entanglement and genuine entanglement of three-qubit Greenberger-Horne-Zeilinger diagonal states

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Abstract

We analytically prove the necessary and sufficient criterion for the full separability of three-qubit Greenberger-Horne-Zeilinger (GHZ) diagonal states. The corresponding entanglement is exactly calculable for some GHZ diagonal states and is tractable for the others using the relative entropy of entanglement. We show that the biseparable criterion and the genuine entanglement are determined only by the biggest GHZ diagonal element regardless of all the other smaller diagonal elements. We have completely solved the entanglement problems of three-qubit GHZ diagonal states.

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Introduction.—Quantum entanglement, being a special form of quantum superposition, possesses structures and properties intrinsically different from any classical system. This difference depends on the number of particles or states involved in the entanglement. For example, the test of Bell inequality using two-qubit entangled states gives statistical prediction, while the three-qubit Greenberger-Horne-Zeilinger (GHZ) entangled states lead to a conflict with local realism non-statistically [1, 2]. Furthermore, the entangled states of more than two qubits are more complicated because of a complex structure due to different ways the qubits can be entangled [3]. Therefore new characteristic methods for multi-qubit states are necessary to fully understand and interpret their quantum behaviors in quantum mechanics.

Multipartite entanglement right now is at the core of quantum information, and provides a critical resource for quantum secret sharing, quantum error-correcting codes and quantum computation [4, 5]. A potential route to quantum computer is the manipulation of electrons trapped in quantum-dot pairs [6]. Recently, the first step revealing the true scalability of spin-based quantum computing was taken by coherently manipulating three individual electron spins confined in neighboring quantum dots [7], where the exchange interactions between the spins are precisely controlled and entangled three-spin states

are generated. To date, multipartite entanglement has been observed in ion traps [8], photon polarization [9], superconducting phase and circuit qubit systems [10], and nitrogen-vacancy centers in diamond [11]. Due to detrimental decoherence effects and imperfections in preparation, the multipartite entangled states prepared are usually mixed, typically, so called GHZ diagonal states. With the experimental realizations, a general separable criterion for GHZ mixed states is important and desired.

One of the key issues is to determine whether the prepared states are genuinely entangled or not entangled at all. Theoretical research has concentrated on the separability and biseparability that characterize the entanglement of the GHZ diagonal states [12, 13, 14, 15, 16, 17, 18]. The criterion for biseparability of three and four-qubit GHZ diagonal states have recently been proved in the form of an inequality involving several density matrix elements in the computational basis [13]. We will show that this criterion can be simplified to the largest GHZ diagonal component being equal or less than $1/2$. This is a significant step that leads to the quantification of genuine entanglement. For the full separability of three-qubit GHZ diagonal states, the sufficient criterion is proposed by directly constructing the fully separable states [17] and the necessary criterion is proposed by the method of convex combinations [18]. Numerical results strongly indicate that the two criteria should coincide. However, it is inconclusive in the absence of an analytical proof.

In this letter, we will prove the unification of the criteria for full separability. The full separability and biseparability provide a practical and accurate method for complete classification of three-qubit GHZ diagonal states, which now can be made into three categories: separable, entangled, and genuinely entangled states discriminated by full separability and biseparability, respectively. In addition to the complete entanglement structure of three-qubit GHZ diagonal states, we also find a new group of entangled states due to the cooperation of the off-diagonal elements in computational basis. This cooperative entanglement may not be detected by the commonly used positive partial transpose (PPT) criterion [19]. We will give the formula

of genuine entanglement and reduce the quantification of entanglement to algebraic calculations.

Necessary and sufficient condition of fully separable three-qubit GHZ states. —The three-qubit GHZ diagonal states take the form

$$\rho = \sum_{k=1}^8 p_k |GHZ_k\rangle \langle GHZ_k|, \quad (1)$$

where the p_k form a probability distribution. The GHZ state basis consists of eight vectors $|GHZ_k\rangle = \frac{1}{\sqrt{2}}(|0x_2x_3\rangle \pm |1\bar{x}_2\bar{x}_3\rangle)$, with $x_i, \bar{x}_i \in \{0, 1\}$ and $x_i \neq \bar{x}_i$. In the binary notation, $k-1 = 0x_2x_3$ for the '+' states and $k-1 = 1\bar{x}_2\bar{x}_3$ for the '-' states. Using Pauli matrices X, Y, Z and 2×2 identity matrix I , the GHZ diagonal states can be written as

$$\rho = \frac{1}{8} [III + \lambda_2 ZZI + \lambda_3 ZIZ + \lambda_4 IZZ + \lambda_5 XXX + \lambda_6 YYX + \lambda_7 YXY + \lambda_8 XYY], \quad (2)$$

where tensor product symbols are omitted.

The sufficient condition of full separability of ρ is [18]

$$1 - |\lambda_-| - \mu \geq 0, \quad (3)$$

or

$$1 - |\lambda_-| - |\lambda_5| - |\lambda_6| - |\lambda_7| - |\lambda_8| \geq 0 \quad (4)$$

where $\lambda_- = \min\{\lambda_2 + \lambda_3 + \lambda_4, \lambda_2 - \lambda_3 - \lambda_4, -\lambda_2 + \lambda_3 - \lambda_4, -\lambda_2 - \lambda_3 + \lambda_4\}$, and

$$\mu = \frac{\sqrt{(\lambda_5\lambda_6 + \lambda_7\lambda_8)(\lambda_5\lambda_7 + \lambda_6\lambda_8)(\lambda_5\lambda_8 + \lambda_6\lambda_7)}}{\sqrt{\lambda_5\lambda_6\lambda_7\lambda_8}}. \quad (5)$$

The sufficient condition comes from an explicit construction of ρ in a fully separable manner [17] [18].

Let us consider the 8×8 density matrix ρ with entries ρ_{ij} in the basis $|000\rangle, |001\rangle, \dots, |111\rangle$ which are ordered in the canonical way. For GHZ diagonal states, the only nonzero elements of ρ are ρ_{ii} and $\rho_{i,9-i}$ ($i = 1, \dots, 8$), and further we have $\rho_{ii} = \rho_{9-i,9-i}$.

The necessary condition for the full separability of GHZ diagonal state ρ [18] can be written as

$$|\mathcal{L}(\rho, \vec{X})| \leq C(\vec{X})\kappa \quad (6)$$

where $\kappa = \min\{\rho_{ii} \ (1 \leq i \leq 4)\}$, $\vec{X} = (\delta, \alpha, \beta, \gamma)$ is a real vector, $\mathcal{L}(\rho, \vec{X}) = \delta\rho_{18} + \alpha\rho_{27} + \beta\rho_{36} + \gamma\rho_{54}$, and

$$C(\vec{X}) = \sup_{a,b,c} [\delta \cos(a+b+c) + \alpha \cos(a) + \beta \cos(b) + \gamma \cos(c)]. \quad (7)$$

Here a, b, c are the angles. The relationship among the density matrix entries ρ_{ij} and the parameters λ_k of a GHZ diagonal state is a simple linear transformation:

$$(\lambda_5, -\lambda_6, -\lambda_7, -\lambda_8) = 4(\rho_{18}, \rho_{36}, \rho_{27}, \rho_{54})H_2, \quad (8)$$

$$\kappa = (1 - |\lambda_-|)/8, \quad (9)$$

where H_2 is the 4×4 Hadamard matrix. Consider the trivial case that \vec{X} is a positive vector, $C(\vec{X})$ achieves its maximum $\delta + \alpha + \beta + \gamma$ when $a = b = c = 0$. If the off-diagonal elements of ρ are all positive, the left-hand side of inequality (6) is the probability mixture of the off-diagonal elements. If two of the off-diagonal elements $\rho_{18}, \rho_{27}, \rho_{36}, \rho_{54}$ are negative, the state can be transformed to a state with all positive off-diagonal elements by local operations and classical communication (LOCC). For these cases, the inequality (6) can be rewritten as

$$\max\{|\rho_{i,9-i}|, (1 \leq i \leq 4)\} \leq \min\{\rho_{ii}, (1 \leq i \leq 4)\}. \quad (10)$$

It is just the PPT criterion. In the case of even number of negative $\rho_{18}, \rho_{27}, \rho_{36}, \rho_{54}$, namely $\prod_{i=5}^8 \lambda_i \leq 0$, PPT criterion is necessary and sufficient for the full separability [17].

What left is to show that if the inequality (3) can be derived from (6) or vice versa when $\prod_{i=5}^8 \lambda_i > 0$. When one of the components of \vec{X} is negative (for definiteness, one may choose $\gamma < 0$), the solutions have been obtained [18] for the angles a, b, c to optimize $C(\vec{X})$ for any given coefficients $\delta, \alpha, \beta, \gamma$. The solutions fulfill the following equations derived from (7)

$$\delta \sin d = -\alpha \sin a = -\beta \sin b = |\gamma| \sin c, \quad (11)$$

where $d \equiv a + b + c$. Without loss of generality, we consider the case where $\rho_{18}, \rho_{36}, \rho_{27}$ are non-negative (this is always possible by LOCC), denote $(x, y, z) = (\delta, \alpha, \beta)/|\gamma|$, and define

$$\begin{aligned} f(x, y, z) &\equiv \frac{|\mathcal{L}(\rho, \vec{X})|}{C(\vec{X})\kappa} \\ &= \frac{(x\rho_{18} + y\rho_{36} + z\rho_{27} - \rho_{54})/\kappa}{x \cos d + y \cos a + z \cos b - \cos c}. \end{aligned} \quad (12)$$

For the outmost surface of the full separability set determined by the necessary condition, we have the following equations

$$\frac{\partial f(x, y, z)}{\partial x} = \frac{\partial f(x, y, z)}{\partial y} = \frac{\partial f(x, y, z)}{\partial z} = 0, \quad (13)$$

$$f(x, y, z) = 1. \quad (14)$$

The solution to equations (13) is

$$\rho_{18} = \kappa \cos d, \rho_{36} = \kappa \cos a, \rho_{27} = \kappa \cos b, \rho_{54} = \cos c, \quad (15)$$

where we have used equations (11), (14) and the fact that $d = a + b + c$ and a, b, c, d are functions of x, y, z in equation (13).

Substituting the solution (15) into equation (8) to obtain λ_i ($i = 5, \dots, 8$), and using of (5) and (9), we have

$$\mu = 1 - |\lambda_-|, \quad (16)$$

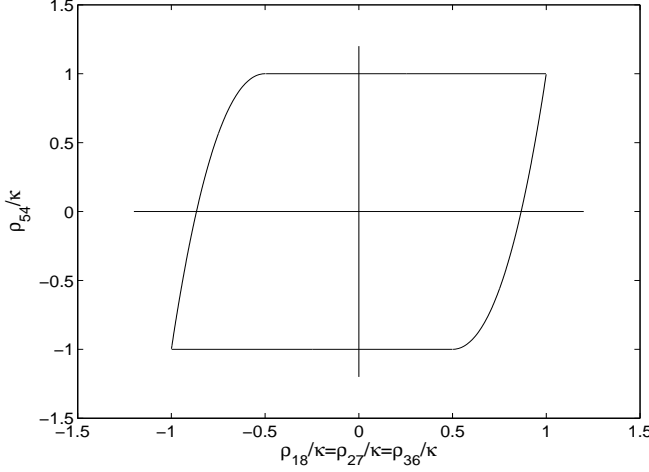


Figure 1: The border curve of full separability

Hence the outmost surface of fully separable state set determined by the necessary condition takes the form of Eq. (16), which is also the outmost surface of fully separable state set determined by the sufficient condition (3). In either odd or even number of negative parameters $\delta, \alpha, \beta, \gamma$, it is shown that the necessary criterion of full separability is also sufficient. Thus we obtain the necessary and sufficient criterion for fully separable of three-qubit GHZ diagonal states.

Consider the case of $\rho_{18} = \rho_{36} = \rho_{27}$, we have the simple solution of $b = a$, $c = -3a$, $d = -a$ ($a \in [0, \pi/3]$) for the border curve of the full separability. More explicitly, we have the equation of border curve

$$\frac{\rho_{54}}{\kappa} = 4\left(\frac{\rho_{18}}{\kappa}\right)^3 - 3\frac{\rho_{18}}{\kappa}. \quad (17)$$

The border curve is shown in Fig.1.

Entanglement:—Entanglement of a given entangled state ρ can be quantified by its relative entropy of entanglement (REE) as, $E = \min_{\sigma \in SEP} S(\rho \parallel \sigma)$, here SEP is the fully separable state set. The relative entropy is defined as, $S(\rho \parallel \sigma) = -\text{Tr} \rho \log_2 \rho + \text{Tr} \rho \log_2 \sigma$. The separable state achieves the minimal relative entropy for state is called its closest state. Follow the same reason given in ref [20], the closest state for a three-qubit GHZ diagonal state ρ must also be a GHZ diagonal state in the form of $\sigma = \sum_{k=1}^8 q_k |GHZ_k\rangle \langle GHZ_k|$, where the q_k form a probability distribution. As the result, the REE can be calculated as,

$$E = \sum_{k=1}^8 p_k \log_2 \left(\frac{p_k}{q_k} \right). \quad (18)$$

The closest state σ is at the boundary of the fully separable states due to the following reasoning: Suppose σ' is an inner state within the fully separable state set. The entangled state ρ is at the outside. A link between σ' and

ρ should intersect with the boundary of the fully separable state set. We have a border state $\sigma = \lambda \sigma' + (1 - \lambda) \rho$ for some $\lambda \in (0, 1)$. Then $S(\rho \parallel \sigma) < \lambda S(\rho \parallel \sigma') + (1 - \lambda) S(\rho \parallel \rho) = \lambda S(\rho \parallel \sigma') < S(\rho \parallel \sigma')$. The first inequality comes from the convexity of negative logarithmic function. Hence an inner separable state is not a closest state. The parameters of a closest state can be written as $q_k = s_k + \kappa_c \cos \theta_k$ and $q_{9-k} = s_k - \kappa_c \cos \theta_k$ for $k = 1, \dots, 4$, where $s_k \geq 0$, $\kappa_c = \min_k \{s_k\}$, $\theta = (d, a, b, c)$. The free variables are a, b, c and three of s_k . We have six free variables and six equations derived from the extremal of (18). REE is tractable. In some special cases, analytical solutions can be obtained as we will show below.

If an entangled GHZ diagonal state ρ has the symmetry of $p_1 = p_2 = p_3$ and $p_6 = p_7 = p_8$, we will prove that the closest state should have the same symmetry of $q_1 = q_2 = q_3$ and $q_6 = q_7 = q_8$. Suppose that a nonsymmetric state $\sigma_1 = \sum_{k=1}^8 q_k |GHZ_k\rangle \langle GHZ_k|$ is the closest state of ρ . By cycling q_1, q_2, q_3 and q_6, q_7, q_8 , we obtain σ_2 and σ_3 which also are closest states of ρ . Let $\bar{\sigma} = \sum_{k=1}^8 \bar{q}_k |GHZ_k\rangle \langle GHZ_k| = \frac{1}{3}(\sigma_1 + \sigma_2 + \sigma_3)$, with $\bar{q}_1 = \bar{q}_2 = \bar{q}_3 = \frac{1}{3}(q_1 + q_2 + q_3)$, $\bar{q}_6 = \bar{q}_7 = \bar{q}_8 = \frac{1}{3}(q_6 + q_7 + q_8)$, then $\bar{\sigma}$ is fully separable since it is a probability mixture of fully separable states. Note that $\frac{1}{3}(q_1 + q_2 + q_3) > \sqrt[3]{q_1 q_2 q_3}$. We have $S(\rho \parallel \bar{\sigma}) < S(\rho \parallel \sigma_1)$, that is a contradiction. The symmetric closest state σ is with $\sigma_{11} = \sigma_{22} = \sigma_{33}$ and $(\sigma_{18}, \sigma_{36}, \sigma_{27}, \sigma_{54}) = \kappa_c (\cos \theta, \cos \theta, \cos \theta, \cos 3\theta)$, where $\theta \in [0, \frac{\pi}{3}]$, and $\kappa_c = \min\{\sigma_{11}, \sigma_{44}\}$. Let $\sigma_{11} = \frac{1}{8} + \frac{1}{3}\xi$, $\sigma_{44} = \frac{1}{8} - \xi$, where $\xi \in [-\frac{3}{8}, \frac{1}{8}]$, we obtain the two optimal equations with variables θ, ξ . The equations are not analytically solvable in general. However, if the closest state is with $\kappa_c = \frac{1}{8}$, exact solution can be obtained. The derivative of (18) on θ leads to

$$\left(\frac{1}{4} - \rho_{11}\right)t^3 - \rho_{18}t^2 - \left(\frac{3}{4} - 4\rho_{11}\right)t + \rho_{18} - \rho_{54} = 0, \quad (19)$$

where $t = 2 \cos \theta$. We then properly choose θ from the three solutions of (19). Note that the derivative of ξ may not exist at $\xi = 0$, we have to calculate the left and right derivatives, which are

$$\begin{aligned} \frac{\partial S(\rho \parallel \sigma)}{\partial \xi} \Big|_{\xi=0^-} &= c_1(\theta) [\cos 3\theta (\cos 3\theta - 8\rho_{54}) + 8\rho_{44} - 1], \\ \frac{\partial S(\rho \parallel \sigma)}{\partial \xi} \Big|_{\xi=0^+} &= c_2(\theta) [\cos \theta (8\rho_{18} - \cos \theta) + 1 - 8\rho_{11}], \end{aligned}$$

where we have used equation (19) to simplify the expressions. $c_1(\theta) = \frac{8}{3 \sin^2 3\theta}$ and $c_2(\theta) = \frac{8(4 \cos^2 \theta - 1)}{\sin^2 3\theta}$ are positive factors for $\theta \in [0, \frac{\pi}{3}]$.

Analytical solutions exist for the states with $\rho_{11} = \rho_{44} = \frac{1}{8}$ when $\theta \in (\frac{\pi}{6}, \frac{\pi}{3}]$. The entanglement can be obtained exactly. We verify that $\cos \theta < 8\rho_{18}$, $\cos 3\theta > 8\rho_{54}$ are true for all the entangled states. The left derivative is negative since $\cos 3\theta < 0$ for $\theta \in (\frac{\pi}{6}, \frac{\pi}{3}]$ and the right derivative is

positive. When $\rho_{54} = -\rho_{18}$, the solution of (19) is $\theta = \frac{\pi}{4}$. The REE is

$$E = \frac{1+8\rho_{18}}{2} \log_2 \frac{1+8\rho_{18}}{1+\frac{1}{\sqrt{2}}} + \frac{1-8\rho_{18}}{2} \log_2 \frac{1-8\rho_{18}}{1-\frac{1}{\sqrt{2}}}.$$

Analytical solutions also exist for states with $\rho_{18} = \rho_{11}$, $\rho_{54} = -\rho_{44}$. Then $p_1 = 2\rho_{11}$, $p_5 = 2\rho_{44}$, $p_4 = p_8 = 0$. We have four kinds of candidate closest states: (i) $\kappa_c = \frac{1}{8}$, (ii) $\kappa_c = \sigma_{1,1} < \frac{1}{8}$, (iii) $\kappa_c = \sigma_{4,4} < \frac{1}{8}$, (iv) PPT boundary state. Here we consider $p_5 > p_1$ (The case $p_5 < p_1$ can be solved similarly). For the first closest state candidate, the relative entropy is simply

$$S(\rho \parallel \sigma) = 3p_1 \log_2 \frac{p_1}{1 + \cos \theta} + p_5 \log_2 \frac{p_5}{1 - \cos 3\theta}. \quad (20)$$

From $\frac{dS(\rho \parallel \sigma)}{d\theta} = 0$, we have $(2 \cos^2 \theta + \Delta \cos \theta - 1)(2 \cos \theta + 1) = 0$, where $\Delta = \frac{p_5 - p_1}{p_5 + p_1}$. The solution is $\cos \theta = \frac{1}{4}(\sqrt{8 + \Delta^2} - \Delta)$. To check that the closest state locates at $\kappa_c = \frac{1}{8}$, we prove that the right derivative is always positive and the left derivative is negative only when $p_1 > p_0 = \frac{1}{12}(3 + \cos 3\theta) \approx 0.1718$. Hence candidate (i) is the solution when $p_1 > p_0$. For $p_1 \leq p_0$, we consider candidate (ii). We have $S(\rho \parallel \sigma) = 3p_1 \log_2 \frac{p_1}{\kappa_c(1 + \cos \theta)} + p_5 \log_2 \frac{p_5}{\frac{1}{2} - \kappa_c(3 + \cos 3\theta)}$. Then $\frac{\partial S(\rho \parallel \sigma)}{\partial \kappa_c} = 0$ gives $\kappa_c = \frac{3p_1}{2(3 + \cos 3\theta)}$. We have

$$S(\rho \parallel \sigma) = 1 + 3p_1 \log_2 \frac{(3 + \cos 3\theta)}{3(1 + \cos \theta)}. \quad (21)$$

The optimal equation is $4 \cos^3 \theta + 6 \cos^2 \theta - 3 = 0$, the solution is $\cos \theta = \frac{1}{2}(\sqrt[3]{2 + \sqrt{3}} + \sqrt[3]{2 - \sqrt{3}} - 1) \approx 0.5979$. The condition $\kappa_c < \frac{1}{8}$ is equivalent to $p_1 < p_0$. The candidate (iii) does not give rise to a further small value of the relative entropy because $\frac{\partial S(\rho \parallel \sigma)}{\partial \kappa_c} < 0$ for all $\theta \in [0, \frac{\pi}{3}]$. The candidate (iv) can also be removed.

Genuine entanglement:—The necessary and sufficient criterion has been proven for biseparability of a three-qubit GHZ diagonal state [13]. It has the form of

$$|\rho_{18}| \leq \sqrt{\rho_{22}\rho_{77}} + \sqrt{\rho_{33}\rho_{66}} + \sqrt{\rho_{44}\rho_{55}}. \quad (22)$$

The criterion can be rewritten as

$$\max\{p_i\} \leq \frac{1}{2}, \quad (23)$$

since for three-qubit GHZ diagonal state, we have $\rho_{ii} = \rho_{9-i,9-i}$, and $p_1 = \rho_{1,1} + |\rho_{1,8}|$. When $p_1 > \frac{1}{2}$, it is followed from the reasoning in the entanglement of the Bell diagonal state [20] that the state is not biseparable. The genuine entanglement measured by REE is $E_{\text{genuine}}(\rho) = \min_{\sigma \in \text{BISEP}} S(\rho \parallel \sigma)$, where *BISEP* is the biseparable state set. Hence

$$E_{\text{genuine}}(\rho) = 1 + p_1 \log_2 p_1 + (1 - p_1) \log_2 (1 - p_1). \quad (24)$$

Also criterion (23) and Eq. (24) are true for four qubit GHZ state as the necessary and sufficient criterion has been proven [13]. The mixture of *N*-qubit GHZ state and white noise is $\rho^{(\text{ghzn})} = (1 - p)|\text{GHZN}\rangle \langle \text{GHZN}| + p\mathbf{1}/2^N$. The state is genuinely entangled iff $0 \leq p < 1/[2(1 - 2^{-N})]$. The probability of $|\text{GHZN}\rangle$ component is $p_1 = (1 - p) + p/2^N = 1 - p(1 - 2^{-N}) > \frac{1}{2}$. The biseparable (yet inseparable under bipartitions) condition can also be written in the form of inequality (23). Therefore its genuine REE can be expressed as Eq.(24).

Summary:—For three-qubit GHZ diagonal state, the fully separable criterion has been strictly proven to be necessary and sufficient. We find the exact boundary states for the fully separable state set. The free variable solution of boundary states make the calculation of the relative entropy of entanglement easy. The relative entropy of entanglement is exactly calculated for the symmetric states ρ ($p_1 = p_2 = p_3, p_6 = p_7 = p_8$) of type (i) $\rho_{ii} = \frac{1}{8}$ ($i = 1, \dots, 8$) (diagonal elements are equal in computational basis) and type (ii) $p_4 = p_8 = 0$. The closest states σ can be either with $\sigma_{ii} = \frac{1}{8}$ ($i = 1, \dots, 8$) or not for both type (i) and type (ii) entangled states. There are many subtleties in obtaining the closest states due to the possible non-existence of the derivative of the relative entropy. We also give the genuine entanglement of GHZ diagonal states in terms of the relative entropy of entanglement. The genuine entanglement is determined by the biggest GHZ diagonal component only. The genuine entanglement formula obtained is easily extended to *N* particle GHZ diagonal states. The fully separable criterion can be applied as a necessary criterion for the separability of any three-qubit state by filtering it to a GHZ diagonal state. Further works on the separability and entanglement of more than three qubit GHZ diagonal states are desirable.

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